Simulation of a Jet Diffusion Flame using Lagrangian Thermal Elements

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Overview

An obstacle to the accurate simulation of the combustion processes in various turbulent combustion phenomena is the inability to model all scales of interactions on the computational grid. Several modeling strategies are presently used to overcome this obstacle (1). The laminar flamelet approach to combustion appears to provide a means of resolving many of the complexities associated with turbulent combustion. Unfortunately however, problems exist with the temporal and spatial temperature and soot species specifications in heavily sooting and radiating flames (2).

Ideally, any turbulent combustion process should be solved in such a way that the grid resolution is adaptive and provides sufficient resolution for the combustion/reaction processes while requiring less accurate resolution of the large scale convective processes. A Lagrangian formulation of the laminar flamelet approach may circumvent some of the difficulties associated with present turbulent combustion calculations (3).

Theory

One might imagine a Lagrangian method of combustion in which computational fuel elements are released into the large scale flow field. This concept may be justified since the singular issue in most turbulent combustion calculations is the "bookkeeping" of the fuel species through oxidation. A coarse grid Eulerian calculation is used to specify the mean mixture fraction (or extent of mixing with air that any individual fuel element undergoes). The coarse grid Eulerian calculation may also prescribe the local turbulence levels (scalar dissipation) at the location of any material element that originated as fuel species. A computation/look-up table from the element specifies the reaction rate, the amount of fuel remaining, the amount of various products generated from the initial mass of fuel, and the amount of soot generated by the initial mass of fuel. The temperature field may be computed on the Eulerian grid using the heat release rates of the small elements as source terms.

As a first approximation to a calculation in which information flows between the small and large scale processes, it is initially proposed that the sole input to the thermal element (i.e., to the small scale Lagrangian fuel element) be the large scale time variable. The thermal element is assumed to be a fuel sphere surrounded by an abundance of oxidizing air. The reaction process is computed on the element. As time progresses, the fuel is oxidized within the thermal element and various product species are formed. Thus, the fuel mass, products mass, and soot mass are all specified by the small scale processes. At any time, the mean mixture fraction of the element is taken from knowledge of the amount of fuel and product species. The convection time of the element in the large scale is equal to the diffusion time associated with combustion on the small scale. In a convective time of dt, the fuel species has been consumed at a rate specified by the diffusional processes within the element.

Practice

In the course of developing this approach for general applications, various canonical flow fields will be investigated using Lagrangian formulations. Thus, a turbulent jet diffusion flame is modeled using the first approximation of this technique. The combustion is modeled using Lagrangian elements in which a diffusion controlled reaction rate takes place. The flow field is decomposed into solenoidal and irrotational components. The jet solenoidal component is simulated using a two equation turbulence model based upon a GENMIX scheme. The irrotational component of the flow field is specified by the heat release rates specified by the thermal elements. It is important to note that although the solenoidal velocity is steady, the overall jet flow field is unsteady and fully three dimensional.

Particles with a precomputed burning history and self contained combustion field are released into the flow field at the jet inlet. At prescribed computational times, new particles enter the flow while older particles are convected downstream into the field. The conserved scalar field of the flame is determined by calculating the local mixture fraction of the individual elements and then interpolating these values onto the Eulerian grid. The various species mass fractions are also interpolated onto the Eulerian mesh in a similar fashion. The temperature field shown below is calculated by interpolating the individual particle temperatures onto the mesh. It is emphasized that an Eulerian or smooth temperature field can also be specified by computation of the energy equation on the Eulerian mesh. The temperature field specified by interpolation of the particle temperatures onto the mesh is relatively hot (i.e., the ambient temperature is not seen on the contour plot). This is consistent with the notion that only particles that originate from the fuel species are being tracked. These particles have recently

burned and are hot. A computation of the energy equation on the Eulerian mesh would provide the more often seen temperature profile with cool ambient temperatures. The results of these preliminary computations indicate that a Lagrangian modeling methodology may be appropriate for some turbulent combustion simulations. The next step is to further couple the mixing rates specified by the large scale processes to the combustion state within the local element.

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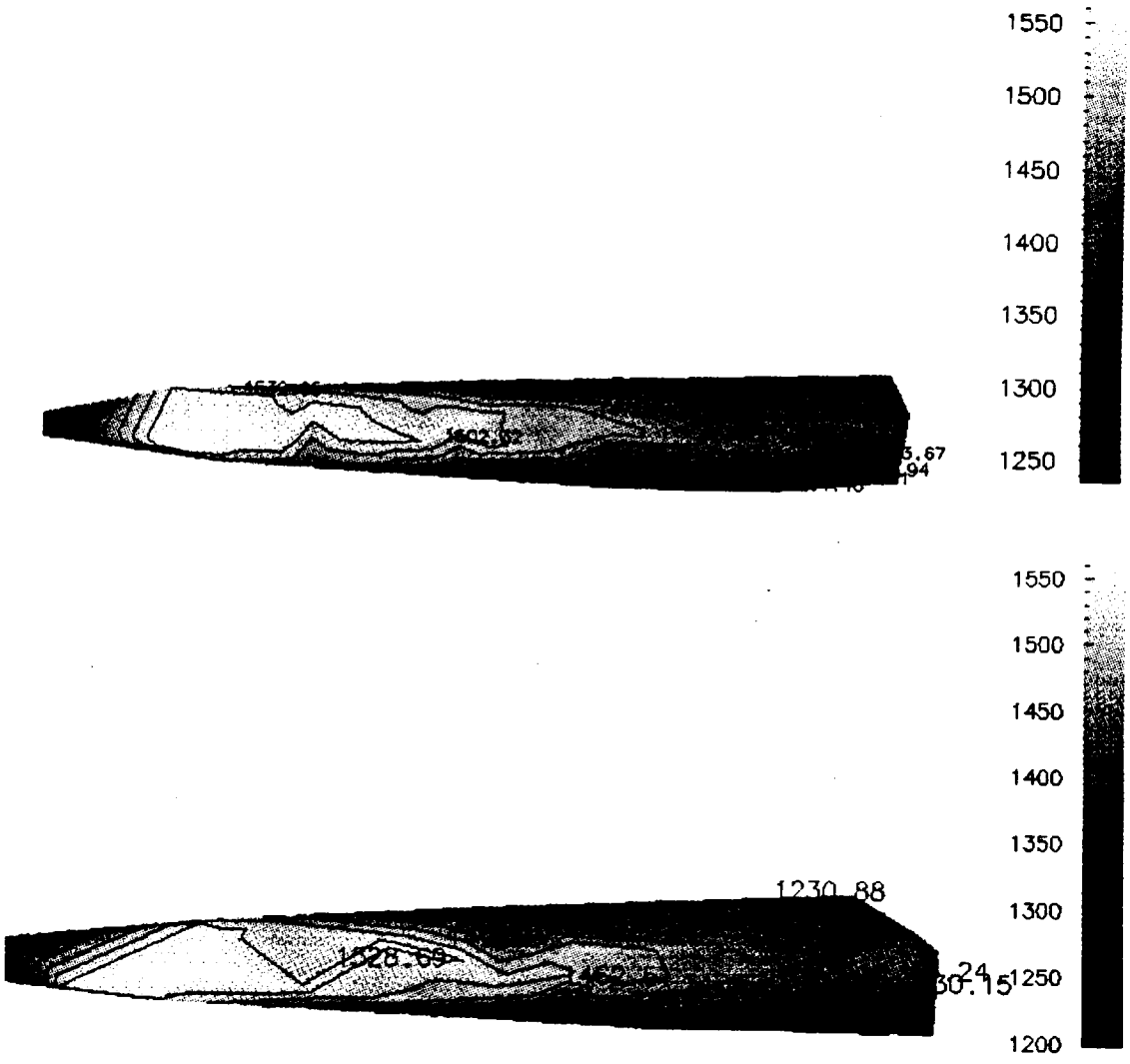

Figure 1. Isotherms at jet cross-section (Re= 20,000): a) t=0.6 seconds after "ignition", b) t= 0.8 seconds after "ignition".